

OFFICE OF NAVAL RESEARCH

CONTRACT N00014-97-1-0066

R&T Code 33e 1806

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Technical Report No. 99

COMPUTED HEATS OF FORMATION

by

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August 13, 1997

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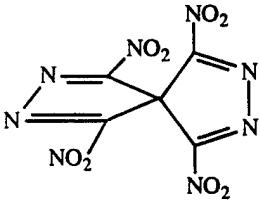
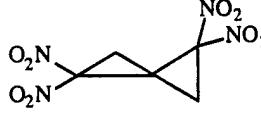
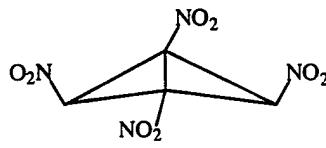
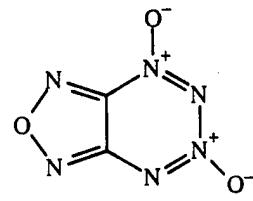
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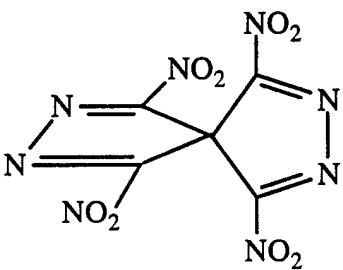
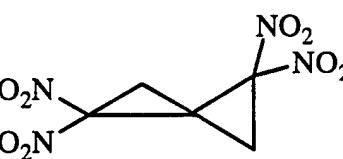
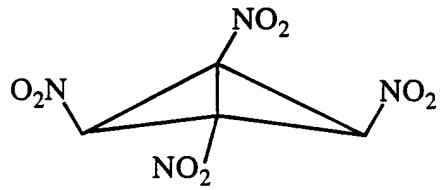
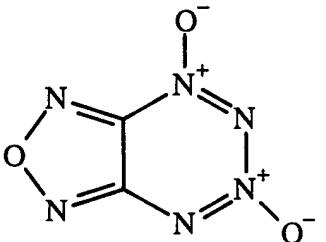
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1. AGENCY USE ONLY (Leave blank)	2. REPORT DATE	3. REPORT TYPE AND DATES COVERED	
	8/13/97	Technical	
4. TITLE AND SUBTITLE		5. FUNDING NUMBERS	
Computed Heats of Formation		N00014-97-1-0066	
6. AUTHOR(S)		Dr. Richard S. Miller	
Peter Politzer, M. Edward Grice and Pat Lane		R&T Code 33e 1806	
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)		8. PERFORMING ORGANIZATION REPORT NUMBER	
University of New Orleans Department of Chemistry New Orleans, Louisiana 70148		99	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)		10. SPONSORING/MONITORING AGENCY REPORT NUMBER	
Office of Naval Research Code 333 800 N. Quincy Street Arlington, VA 22217			
11. SUPPLEMENTARY NOTES			
12a. DISTRIBUTION / AVAILABILITY STATEMENT		12b. DISTRIBUTION CODE	
Approved for public release. Unlimited distribution.			
13. ABSTRACT (Maximum 200 words) Computed heats of formation for 1 - 4.			
   			
1: ΔH_f^{298K} (solid) = 157 kcal/mole = 524 cal/g		3: ΔH_f^{298K} (solid) = 59 kcal/mole = 250 cal/g	
2: ΔH_f^{298K} (solid) = 46 kcal/mole = 183 cal/g		4: ΔH_f^{298K} (solid) = 143 kcal/mole = 918 cal/g	
14. SUBJECT TERMS		15. NUMBER OF PAGES	
energetic compounds; heats of formation		4	
		16. PRICE CODE	
17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
Unclassified	Unclassified	Unclassified	Unlimited

We have used our density functional procedure [1] to compute the heats of formation of the compounds **1 - 4**, in response to a request from R. Naylor (Allegany Ballistics Laboratory). The vibrational energies were determined from the molecular stoichiometries [2]. The density functional calculations give the gas phase heat of formation, which we convert to the liquid and solid state values by subtracting, respectively, the heat of vaporization and the heat of sublimation. These are obtained by means of relationships that we have developed involving the computed electrostatic potential on the molecular surface [3,4].

Results:

1 	ΔH_f^{298K} (gas) = 189 kcal/mole = 630 cal/g ΔH_f^{298K} liquid = 174 kcal/mole = 579 cal/g ΔH_f^{298K} (solid) = 157 kcal/mole = 524 cal/g
2 	ΔH_f^{298K} (gas) = 76 kcal/mole = 304 cal/g ΔH_f^{298K} liquid = 60 kcal/mole = 243 cal/g ΔH_f^{298K} (solid) = 46 kcal/mole = 183 cal/g
3 	ΔH_f^{298K} (gas) = 85 kcal/mole = 364 cal/g ΔH_f^{298K} liquid = 71 kcal/mole = 303 cal/g ΔH_f^{298K} (solid) = 59 kcal/mole = 250 cal/g
4 	ΔH_f^{298K} (gas) = 165 kcal/mole = 1058 cal/g ΔH_f^{298K} liquid = 152 kcal/mole = 974 cal/g ΔH_f^{298K} (solid) = 143 kcal/mole = 918 cal/g

For comparison, the experimental gas phase ΔH_f^{298K} value for RDX is 206 cal/g [5,6].

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